Direct spectroscopic calculations in the framework of the information system "Spectroscopy of Atmospheric Gases"

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The paper describes a direct spectroscopic line parameter calculation, which has been included as a user-accessible function of the information system "Spectroscopy of Atmospheric Gases." The system offers an Internet access to commonly used spectroscopic compilations HITRAN and GEISA as well as to original databanks. The theoretical models employed for this option are briefly outlined including those of effective Hamiltonians and moments for dipole transitions. A thorough description of input spectroscopic parameters, as well as parameters determining the conditions for calculating spectra, is presented.

Introduction

An information-computing system SPECTRA ("Spectroscopy of Atmospheric Gases") is under development in the Laboratory of Theoretical Spectroscopy of the Institute of Atmospheric Optics of Russian Academy of Science since 1999. It provides an Internet access to information on spectral line parameters (SLP) and absorption cross sections for atmospheric gases, as well as assists at some standard tasks of molecular spectroscopy. Among these tasks, a user has an access to: (1) search, selection, and visualisation of SLP, (2) modeling laboratory spectra of low and high resolution, and (3) direct spectroscopic calculations based on the method of effective operators (Hamiltonians and transition moment). A general composition and the structure of the system were described in Ref. 1. Additional information on the system, its user options and functions can be found in the "info" section of the SPECTRA itself.

As for the SLP base, the system can read line parameters available in the well-known databases HITRAN-2000 (including additions of 2001),[2] HITEMP,[3] and GEISA.[4] At the latest version, the system has an access to original SLP obtained by several research teams which are not yet present at other commonly accessible banks of spectroscopic information, in particular, extended data for the water vapor, carbon dioxide,[5,6] and hydrogen sulphide.[7] Theoretical line parameters of 6 isotopic water species have been reproduced using the original method and data.[8,9] Many of the original data have been obtained within cooperation projects between the Institute of Atmospheric Optics SB RAS and some leading spectroscopy research teams of USA and France.

The home page of SPECTRA is shown in Fig. 1. Note that though a registration is not obligatory, the registered users have an access to a larger number of options and services. All graphical and computational results available on the http://spectra.iao.ru cite can be saved in personal databases on the server within a limited quotas of a disk space or at a user's computer, or be sent to the user via e-mail as attached text files for a further processing.

The section "Direct spectroscopic calculations" allows a user to carry out his own calculations for the water molecule and for open configuration of the ozone molecule using input parameters of the Hamiltonian and transition moment operator. Both belong to triatomic molecules of the asymmetric top type. A calculation of vibration-rotation (VR) spectra of these molecules is carried out using the computer program GIP ("General Inverse Problem").[10] In the next section we give a general description for this information system function. The corresponding page of SPECTRA is shown in Fig. 2. We draw attention to theoretical model and to the definition of their parameters used in the system.

Theoretical models

The computer program GIP[10] has been developed as a tool for direct and inverse (data fitting) calculations of high-resolution molecular spectroscopy. It allows calculating energies and wave functions of VR states and also frequencies and intensities of rotational-vibrational (RV) transitions. In this paper we describe only a version of this code designed for calculations of asymmetric top spectra. The program has been used in many analyses of VR spectra for fitting of energy levels, line positions, and intensities of water[11-13] and ozone[14-18] molecules. The calculation is based on the method of effective Hamiltonians and effective transition moment operators.
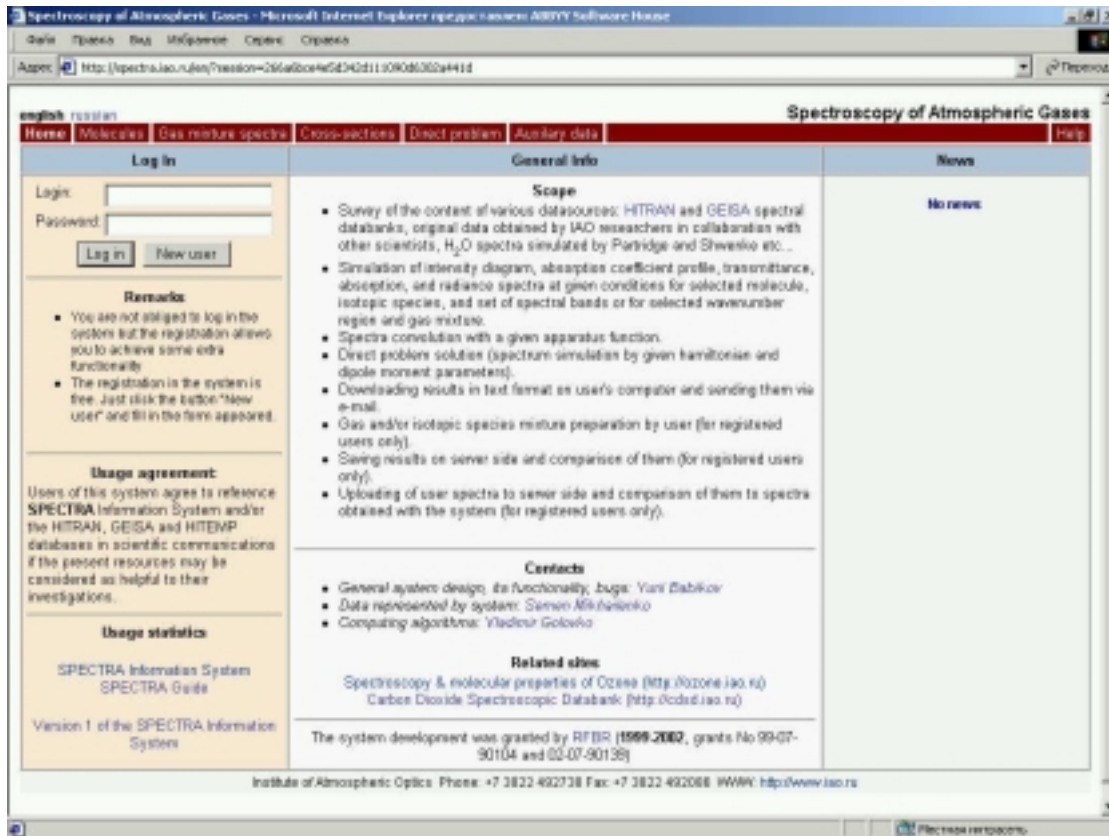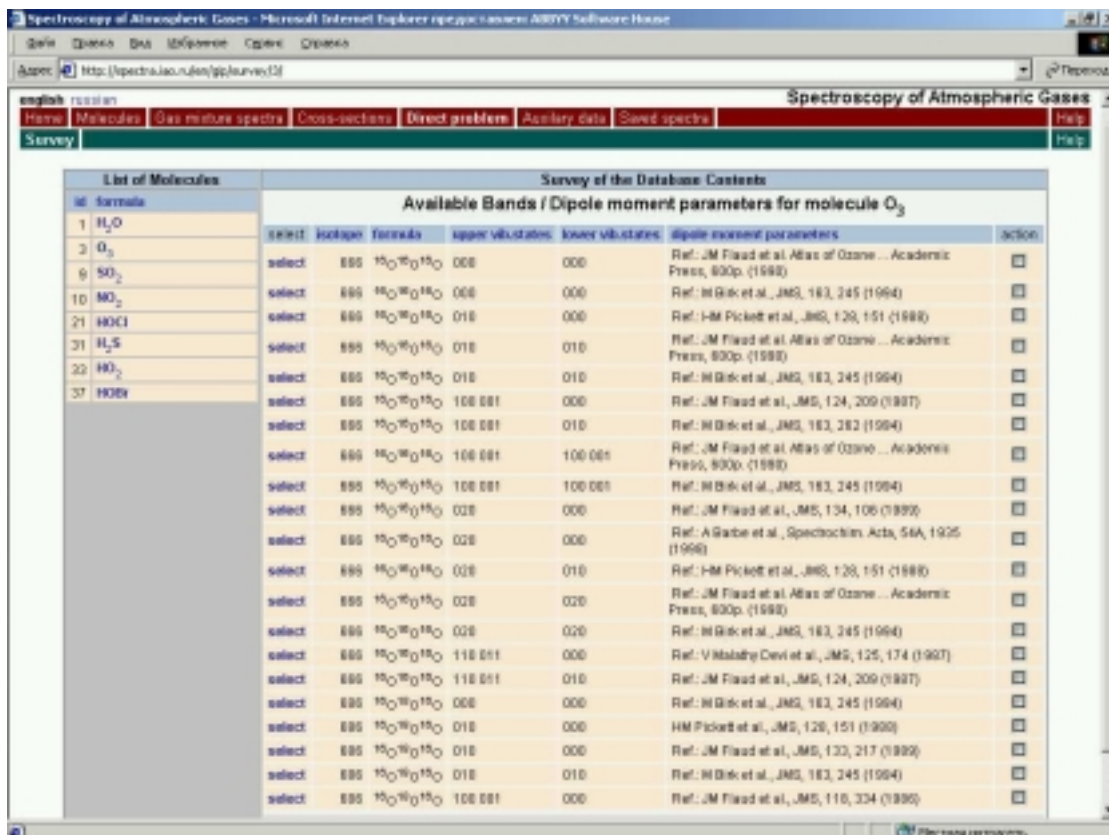
Fig. 1. The home page of SPECTRA.

Fig. 2. A window containing the list of VR ozone bands, for which the direct calculation function is operational at the moment.

Effective transition moment operators

Following the theory of line intensities of non-rigid asymmetric top molecules,[19,20] one needs to calculate matrix elements of transformed dipole moment operator

$$^{VV'}\mathbf{\mu}_Z = \sum_k {}^{VV'}\mu_k \mathbf{A}_k, \tag{1}$$

in order to compute RV line intensities. Here numerical coefficients $^{VV'}\mu_k$ parametrise the effective dipole transition moment operator for the corresponding band. Each vibrational band is defined by a set of lower and upper vibration quantum numbers $V \equiv (V_1 V_2 V_3)$. Parameters $^{VV'}\mu_k$ can be found from a fit of experimental data, this procedure being called inverse spectroscopic calculation. Combinations of rotational operators $\mathbf{A}_k$ depend on the type of vibrational transition. The following notations[20] are used for the operator (1):

a) for A-type bands (ΔV_3 odd)

$$\mathbf{\mu}_Z = \mu_1 \phi_z + \mu_2 \{\phi_z, \mathbf{J}^2\} + \mu_3 \{\phi_z, \mathbf{J}_z^2\} +$$

$$+ \mu_4 \frac{1}{2}[\{\phi_x, i\mathbf{J}_y\} - \{i\phi_y, \mathbf{J}_x\}] +$$

$$+ \mu_5 \frac{1}{2}[\{\phi_x, \{\mathbf{J}_x, \mathbf{J}_z\}\} - \{i\phi_y, \{i\mathbf{J}_y, \mathbf{J}_z\}\}] +$$

$$+ \mu_6 \frac{1}{2}[\{\phi_x, i\mathbf{J}_y\} + \{i\phi_y, \mathbf{J}_x\}] +$$

$$+ \mu_7 \frac{1}{2}[\{\phi_x, \{\mathbf{J}_x, \mathbf{J}_z\}\} + \{i\phi_y, \{i\mathbf{J}_y, \mathbf{J}_z\}\}] + \mu_8 \{\phi_z, \mathbf{J}_{xy}^2\}; \tag{2}$$

b) for B-type bands (ΔV_3 even)

$$\mathbf{\mu}_Z = \mu_1 \phi_x + \mu_2 \{\phi_x, \mathbf{J}^2\} + \mu_3 \{\phi_x, \mathbf{J}_z^2\} +$$

$$+ \mu_4 \{i\phi_y, \mathbf{J}_z\} + \mu_5 \{\phi_z, i\mathbf{J}_y\} + \mu_6 \{\phi_z, \{\mathbf{J}_x, \mathbf{J}_z\}\} +$$

$$+ \mu_7 \frac{1}{2}[\{\phi_x, \mathbf{J}_{xy}^2\} - \{i\phi_y, \{\mathbf{J}_x, i\mathbf{J}_y\}\}] +$$

$$+ \mu_8 \frac{1}{2}[\{\phi_x, \mathbf{J}_{xy}^2\} + \{i\phi_y, \{\mathbf{J}_x, i\mathbf{J}_y\}\}]. \tag{3}$$

For simplicity, left superindices of the operator $^{VV'}\mu_Z$ and parameters $^{VV'}\mu_k$ are omitted in Eqs. (2) and (3). Other notations are standard: $\mathbf{J}_x$, $\mathbf{J}_y$, $\mathbf{J}_z$ stand for molecular frame components of the angular momentum

$$\mathbf{J}^2 = \mathbf{J}_x^2 + \mathbf{J}_y^2 + \mathbf{J}_z^2, \;\; \mathbf{J}_{xy}^2 = \mathbf{J}_x^2 - \mathbf{J}_y^2$$

$$\text{and } \{\mathbf{A}, \mathbf{B}\} = \mathbf{AB} + \mathbf{BA}.$$

Expressions for direction cosines matrix elements ϕ_α ($\alpha = x, y, z$) can be found in Ref. 20.

Rotational terms in effective Hamiltonians

To represent effective rotational Hamiltonians for the ozone molecule, the standard Watson form[21]

is currently used. In the case of $^{16}O^{18}O^{16}O$ isotopic species it was sufficient to include 36 terms in this Hamiltonian

$$\mathbf{H}_V^{\text{Wats}} = E^V + [A^V - \frac{1}{2}(B^V + C^V)]\mathbf{J}_z^2 + \frac{1}{2}(B^V + C^V)\mathbf{J}^2 +$$

$$+ \frac{1}{2}(B^V - C^V)\mathbf{J}_{xy}^2 - \Delta_K^V \mathbf{J}_z^4 - \Delta_{JK}^V \mathbf{J}^2 \mathbf{J}_z^2 -$$

$$- \Delta_J^V \mathbf{J}^4 - \delta_K^V \{\mathbf{J}_z^2, \mathbf{J}_{xy}^2\} - 2\delta_J^V \mathbf{J}^2 \mathbf{J}_{xy}^2 + H_K^V \mathbf{J}_z^6 + H_{KJ}^V \mathbf{J}^2 \mathbf{J}_z^4 +$$

$$+ H_{JK}^V \mathbf{J}^4 \mathbf{J}_z^2 + H_J^V \mathbf{J}^6 + h_K^V \{\mathbf{J}_z^4, \mathbf{J}_{xy}^2\} +$$

$$+ h_{JK}^V \mathbf{J}^2 \{\mathbf{J}_z^2, \mathbf{J}_{xy}^2\} + 2h_J^V \mathbf{J}^4 \mathbf{J}_{xy}^2 + L_K^V \mathbf{J}_z^8 +$$

$$+ L_{KJ}^V \mathbf{J}^2 \mathbf{J}_z^6 + L_{KKJ}^V \mathbf{J}^4 \mathbf{J}_z^4 + L_{JK}^V \mathbf{J}^6 \mathbf{J}_z^2 + L_J^V \mathbf{J}^8 +$$

$$+ l_K^V \{\mathbf{J}_z^6, \mathbf{J}_{xy}^2\} + l_{KJ}^V \mathbf{J}^2 \{\mathbf{J}_z^4, \mathbf{J}_{xy}^2\} + l_{JK}^V \mathbf{J}^4 \{\mathbf{J}_z^2, \mathbf{J}_{xy}^2\} +$$

$$+ 2l_J^V \mathbf{J}^6 \mathbf{J}_{xy}^2 + P_K^V \mathbf{J}^{10} + P_{KJ}^V \mathbf{J}^2 \mathbf{J}_z^8 + P_{KKJ}^V \mathbf{J}^4 \mathbf{J}_z^6 +$$

$$+ P_{JJK}^V \mathbf{J}^6 \mathbf{J}_z^4 + P_{JK}^V \mathbf{J}^8 \mathbf{J}_z^2 + P_J^V \mathbf{J}^{10} + p_K^V \{\mathbf{J}_z^8, \mathbf{J}_{xy}^2\} +$$

$$+ p_{KJ}^V \mathbf{J}^2 \{\mathbf{J}_z^6, \mathbf{J}_{xy}^2\} + p_{KKJ}^V \mathbf{J}^4 \{\mathbf{J}_z^4, \mathbf{J}_{xy}^2\} +$$

$$+ p_{JK}^V \mathbf{J}^6 \{\mathbf{J}_z^2, \mathbf{J}_{xy}^2\} + 2p_J^V \mathbf{J}^8 \mathbf{J}_{xy}^2 \tag{4}$$

with the same notations for rotational operators as in Eqs. (2) and (3). Coefficients associated with various operators in the expansion (4) are usually called Watson spectroscopic parameters.

For the major isotopologue of ozone $^{16}O_3$ a more extended expansion of the Hamiltonian was used in the literature, including terms corresponding to the 12th power of angular momentum components with a total of 49 parameters. For this molecule we use a representation of angular momentum operator in terms of cylindrical components $\mathbf{J}_+ = \mathbf{J}_x - i\mathbf{J}_y$ and $\mathbf{J}_- = \mathbf{J}_x + i\mathbf{J}_y$. The 25 lower order terms of the operator (4) in this representation take the following form:

$$\mathbf{H}_V^{\text{Wats}} = E^V + [A^V - \frac{1}{2}(B^V + C^V)]\mathbf{J}_z^2 + \frac{1}{2}(B^V + C^V)\mathbf{J}^2 +$$

$$+ \frac{1}{4}'(B^V - C^V)(\mathbf{J}_+^2 + \mathbf{J}_-^2) - \Delta_K^V \mathbf{J}_z^4 -$$

$$- \Delta_{JK}^V \mathbf{J}^2 \mathbf{J}_z^2 - \Delta_J^V \mathbf{J}^4 + '\delta_K^V [\mathbf{J}_+^2 (\mathbf{J}_z + 1)^2 + (\mathbf{J}_z + 1)^2 \mathbf{J}_-^2] +$$

$$+ '\delta_J^V \mathbf{J}^2 (\mathbf{J}_+^2 + \mathbf{J}_-^2) + H_K^V \mathbf{J}_z^6 + H_{KJ}^V \mathbf{J}^2 \mathbf{J}_z^4 +$$

$$+ H_{JK}^V \mathbf{J}^4 \mathbf{J}_z^2 + H_J^V \mathbf{J}^6 + 'h_K^V [\mathbf{J}_+^2 (\mathbf{J}_z + 1)^4 + (\mathbf{J}_z + 1)^4 \mathbf{J}_-^2] +$$

$$+ 'h_{JK}^V \mathbf{J}^2 [\mathbf{J}_+^2 (\mathbf{J}_z + 1)^2 + (\mathbf{J}_z + 1)^2 \mathbf{J}_-^2] +$$

$$+ 'h_J^V \mathbf{J}^4 [\mathbf{J}_+^2 + \mathbf{J}_-^2] + L_K^V \mathbf{J}_z^8 + L_{KJ}^V \mathbf{J}^2 \mathbf{J}_z^6 + L_{KKJ}^V \mathbf{J}^4 \mathbf{J}_z^4 +$$

$$+ L_{JK}^V \mathbf{J}^6 \mathbf{J}_z^2 + L_J^V \mathbf{J}^8 + 'l_K^V [\mathbf{J}_+^2 (\mathbf{J}_z + 1)^6 + (\mathbf{J}_z + 1)^6 \mathbf{J}_-^2] +$$

$$+ 'l_{KJ}^V \mathbf{J}^2 [\mathbf{J}_+^2 (\mathbf{J}_z + 1)^4 + (\mathbf{J}_z + 1)^4 \mathbf{J}_-^2] + 'l_{JK}^V \mathbf{J}^4 [\mathbf{J}_+^2 (\mathbf{J}_z + 1)^2 +$$

$$+ (\mathbf{J}_z + 1)^2 \mathbf{J}_-^2] + 'l_J^V \mathbf{J}^6 [\mathbf{J}_+^2 + \mathbf{J}_-^2] + \dots . \tag{5}$$

In order to match the parameters of the latter representations with original Watson parameters, one needs to consider linear combinations for rotationally non-diagonal terms $1/2(B^V - C^V)$, δ_K^V, δ_J^V, h_K^V, h_{JK}^V, h_J^V, etc. To distinguish the corresponding parameters in two representations, the latter ones are usually noted with primes. For example, the first "primed" parameter of Eq. (5) is related with Watson parameters as follows:

$$\frac{1}{4}'(B^V - C^V) = \frac{1}{4}(B^V - C^V) - \delta_K^V + h_K^V + l_K^V + p_K^V + q_K^V.$$

The parameter q_K^V in the latter equation corresponds to the operator $\{\mathbf{J}_z^{10}, \mathbf{J}_{xy}^2\}$. Relations for the following 14 non-diagonal in the rotational basis terms of the Hamiltonian are given in Table 1.

Table 1. Relation between rotationally non-diagonal parameters of the operator (5) and Watson centrifugal distortion parameters

Parameter number	Operator in Eq. (5)	Expression*
2	$'\delta_J^V$	$-\delta_J^V + h_{JK}^V + l_{KJ}^V + p_{KJ}^V + q_{KJ}^V$
3	$'\delta_K^V$	$-\delta_K^V + 6h_K^V + 15l_K^V + 28p_K^V + 45q_K^V$
4	$'h_K^V$	$h_K^V + 15l_K^V + 70p_K^V + 210q_K^V$
5	$'h_{JK}^V$	$h_{JK}^V + 6l_{KJ}^V + 15p_{KJ}^V + 28q_{KJ}^V$
6	$'h_J^V$	$h_J^V + l_{JK}^V + p_{KKJ}^V + q_{KKJ}^V$
7	$'l_K^V$	$l_K^V + 28p_K^V + 210q_K^V$
8	$'l_{KJ}^V$	$l_{KJ}^V + 15p_{KJ}^V + 70q_{KJ}^V$
9	$'l_{JK}^V$	$l_{JK}^V + 6p_{KKJ}^V + 15q_{KKJ}^V$
10	$'l_J^V$	$l_J^V + p_{JK}^V + q_{JJK}^V$
11	$'p_K^V$	$p_K^V + 45q_K^V$
12	$'p_{KJ}^V$	$p_{KJ}^V + 28q_{KJ}^V$
13	$'p_{KKJ}^V$	$p_{KKJ}^V + 15q_{KKJ}^V$
14	$'p_{JK}^V$	$p_{JK}^V + 6q_{JJK}^V$
15	$'p_J^V$	$p_J^V + q_{JK}^V$

* Parameter q_{KJ}^V corresponds to operator $\mathbf{J}^2\{\mathbf{J}_z^8, \mathbf{J}_{xy}^2\}$, parameter q_{KKJ}^V corresponds to operator $\mathbf{J}^4\{\mathbf{J}_z^6, \mathbf{J}_{xy}^2\}$, parameter q_{JJK}^V corresponds to operator $\mathbf{J}^6\{\mathbf{J}_z^4, \mathbf{J}_{xy}^2\}$, parameter q_{JK}^V corresponds to operator $\mathbf{J}^8\{\mathbf{J}_z^2, \mathbf{J}_{xy}^2\}$, parameter q_J^V corresponds to operator $\mathbf{J}^{10}\mathbf{J}_{xy}^2$.

As is well known (see, for example, Refs. 11–13, 22–24), for a correct description of RV levels of non-rigid water type molecules it is necessary to apply more sophisticated models than a standard power series expansions (4) and (5). For this purpose, we employ an effective rotation Hamiltonian expressed in terms of the generating function model.

According to Ref. 11, a rotational Hamiltonian for this model can be written as following:

$$\mathbf{H}_{rot}^G = \sum_m \sum_n g_{nm} \mathbf{J}^{2n} [\mathbf{G}(\boldsymbol{\alpha}^{(J)})]^m +$$

$$+ \sum_m \sum_n u_{nm} \mathbf{J}^{2n} \{(\mathbf{J}_+^2 + \mathbf{J}_-^2), [\mathbf{G}(\boldsymbol{\beta}^{(J)})]^m\}. \quad (6)$$

Summation indices m and n take integer values starting with zero. Coefficients g_{nm} and u_{nm} are considered as spectroscopic parameters and can by found from a fit of experimental line positions or energy levels. As for operators (4) and (5), parameters of the Hamiltonian $\mathbf{H}_{rot}^G$ depend on vibration quantum numbers V, which is omitted for the sake of simplicity. Operators $\mathbf{G}$ are called elementary generating functions. We use for them the following expressions[23]

$$\mathbf{G}(\boldsymbol{\alpha}^{(J)}) = \frac{2}{\boldsymbol{\alpha}^{(J)}}[\sqrt{1 + \boldsymbol{\alpha}^{(J)}\mathbf{J}_z^2} - 1], \quad (7)$$

where

$$\boldsymbol{\alpha}^{(J)} = \alpha_0 + \alpha_1 \mathbf{J}^2 + \alpha_2 \mathbf{J}^4 + \alpha_3 \mathbf{J}^6 + \alpha_4 \mathbf{J}^8 + \alpha_5 \mathbf{J}^{10} \quad (7a)$$

and

$$\mathbf{G}(\boldsymbol{\beta}^{(J)}) = \frac{2}{\boldsymbol{\beta}^{(J)}}[\sqrt{1 + \boldsymbol{\beta}^{(J)}\mathbf{J}_z^2} - 1], \quad (8)$$

where

$$\boldsymbol{\beta}^{(J)} = \beta_0 + \beta_1 \mathbf{J}^2 + \beta_2 \mathbf{J}^4 + \beta_3 \mathbf{J}^6 + \beta_4 \mathbf{J}^8. \quad (8a)$$

The α_i and β_i in the formulae (7a) and (8a) are nonlinear spectroscopic parameters, which are determined from a fit similarly to g_{nm} and u_{nm}. Approximate relations between parameters of the model (6) and Watson spectroscopic parameters can be found in Refs. 11 and 23. Note that the parameter g_{00} corresponds to E^V.

Effective Hamiltonian for a set of strongly interacting vibration states

An approximation of single-state rotational Hamiltonians written separately for various vibration states appears to be non-adequate for a description of observed RV spectra in a case of resonances. A use of above mentioned pure rotational Hamiltonians of the type (4) or (6) does not allow describing resonance perturbations independently of the order of the expansion. In such cases an appropriate effective VR Hamiltonian should be formulated for a set of vibrational states coupled by resonances. First examples of applications of these types of models can be found in Refs. 25–28. In such cases, a notion of "interacting" or "strongly coupled" vibration states (or of corresponding bands) is often used. A model effective Hamiltonian contains then operators which are responsible for these resonance interactions (which correspond to "resonance blocks" discussed below).

For example, for a set of two interacting states the corresponding Hamiltonian can be written in a mixed matrix-operator form of a vibration dimension of 2:

$$\mathbf{H}^{\mathrm{dyad}} = \begin{vmatrix} \mathbf{H}_{V_1} & \mathbf{H}_{V_1V_2}^+ \\ \mathbf{H}_{V_1V_2} & \mathbf{H}_{V_2} \end{vmatrix}. \tag{9}$$

This model has been originally introduced in a semi-empirical way. For our use (having in mind applications to the ozone and water molecules), one can write the diagonal vibrational blocks of Eq. (9) $\mathbf{H}_{V_1}$ and $\mathbf{H}_{V_2}$ in the form (4), (5) or (6) that represent effective rotational Hamiltonian for V_1 and V_2 states. Vibrational off-diagonal operator $\mathbf{H}_{V_1V_2}$ responsible for VR-coupling of states can be approximated as a polynomial in $\mathbf{J}_\alpha$ components. Another off-diagonal block $\mathbf{H}_{V_1V_2}^+$ is obtained by a hermitian conjugation of $\mathbf{H}_{V_1V_2}$. Examples of a use of the model (9) can be found in Refs. 25 and 26.

For three states coupled by resonances an effective VR Hamiltonian can be written as a three by three vibration matrix, where matrix elements are rotational operators

$$\mathbf{H}^{\mathrm{triad}} = \begin{vmatrix} \mathbf{H}_{V_1} & \mathbf{H}_{V_1V_2}^+ & \mathbf{H}_{V_1V_3}^+ \\ \mathbf{H}_{V_1V_2} & \mathbf{H}_{V_2} & \mathbf{H}_{V_2V_3}^+ \\ \mathbf{H}_{V_1V_3} & \mathbf{H}_{V_2V_3} & \mathbf{H}_{V_3} \end{vmatrix}. \tag{10}$$

Similarly to the case of Eq. (9), one sets effective rotational Hamiltonians for diagonal blocks. Off-diagonal blocks represent resonance coupling operators. A Hamiltonian of the form (10) has been used in Ref. 28 to describe rotational levels of the triad of vibration states (020), (100), and (001) of the $H_2^{16}O$ molecule. Operators of the type $\mathbf{H}^{\mathrm{dyad}}$ and $\mathbf{H}^{\mathrm{triad}}$ are called centrifugal distortion Hamiltonians for a polyad of vibration states coupled by resonance interactions.

Resonance coupling operators

Several equivalent terms can be found in the spectroscopic literature to denote a strong VR coupling, which is often called "resonance interaction" or simply "interaction" of vibrational states. More detailed information can be found in Refs. 29–32. Following to the literature, one can distinguish two different types of resonances for asymmetric top molecules:

1. Anharmonic resonances due to resonance interactions of closely lying VR states, which belong to vibrational states of the same symmetry species with a major coupling contribution from the anharmonic part of the molecular potential energy function.

2. Coriolis resonances due to resonance interactions of closely lying VR states, which belong to vibrational states of different symmetry species with a major coupling contribution from the Coriolis part of the VR Hamiltonian.

Here we refer to resonance coupling operators of both types and specify the corresponding input sets of parameters for SPECTRA computations.

A general form of anharmonic resonance blocks follows that of Ref. 33:

$$\mathbf{H}_{VV'} = \mathbf{H}^{\mathrm{Anh}} =$$

$$= \sum_{l\,r\,m} \mathbf{J}^{2l}[\mathbf{J}_+^{2r}(\mathbf{J}_z + r)^m + (-1)^m(\mathbf{J}_z + r)^m \mathbf{J}_-^{2r}]A_{LmR}, \tag{11}$$

where $L = 2l$ and $R = 2r$, all coefficients A_{LmR} being real for molecules of the C_{2V} point group. A present version of the computing code uses 11 terms of Eq. (11):

$$\mathbf{H}^{\mathrm{Anh}} = A_{000} + A_{200}\mathbf{J}^2 + A_{020}\mathbf{J}_z^2 +$$

$$+ A_{002}(\mathbf{J}_+^2 + \mathbf{J}_-^2) + A_{400}\mathbf{J}^4 + A_{040}\mathbf{J}_z^4 + A_{220}\mathbf{J}^2\mathbf{J}_z^2 +$$

$$+ A_{012}[\mathbf{J}_+^2(\mathbf{J}_z + 1) + (\mathbf{J}_z + 1)\mathbf{J}_-^2] + A_{202}\mathbf{J}^2(\mathbf{J}_+^2 + \mathbf{J}_-^2) +$$

$$+ A_{022}[\mathbf{J}_+^2(\mathbf{J}_z + 1)^2 + (\mathbf{J}_z + 1)^2\mathbf{J}_-^2] + A_{004}(\mathbf{J}_+^4 + \mathbf{J}_-^4). \tag{12}$$

A general form of Coriolis resonance blocks is written in the form[34]

$$\mathbf{H}_{VV'} = \mathbf{H}^{\mathrm{Cor}} =$$

$$= \sum_r \sum_{l+m=0}^{r-1} \mathbf{J}^{2l}[\mathbf{J}_+^r(\mathbf{J}_z + r/2)^m + (-1)^m(\mathbf{J}_z + r/2)^m \mathbf{J}_-^r]C_{Lmr}, \tag{13}$$

with real coefficients C_{Lmr} appropriate to our applications. A present version of the computing code uses 20 terms of Eq. (13). Corresponding combinations of indices for parameters are listed in Table 2. Note that Tables 2 and 3 display a complete set of parameters available in the version of GIP program which is implemented in SPECTRA.

Coefficients A_{LmR} and C_{Lmr} of expansions (11) and (13) are often called interaction parameters, or resonance parameters, or coupling parameters for two vibration states. Note that indices corresponding to vibration quantum numbers V and V' were omitted in Eqs. (11)–(13) for the sake of simplicity.

Direct spectroscopic calculation in SPECTRA system

By choosing the case "Direct problem" in the main menu of the SPECTRA system, a user accesses the page shown in Fig. 2. At the left hand side of this page one finds a list of molecules, for which a calculation of VR spectra is accessible in SPECTRA via the GIP computer program. In order to choose a molecule, it is sufficient to click on a corresponding molecular symbol. As it was mentioned, computations for the ozone and water molecules are operational in the present version of the information system. The right-hand side gives the list of bands and parameter sets for transition moments (2) and (3) for a chosen molecule. A detailed description of various records

Table 2. Spectroscopic parameters (cm^{-1}) of Hamiltonian H^{dyad} for interacting vibrational states (100) and (001) of ^{16}O^{18}O^{16}O molecule[35]

Parameter number	Parameter	(100) Value	(001) Value
1	(B–C)/2	.270479650E–01	.266322800E–01
2	–dj	–.729000000E–07	–.771380000E–07
3	hj	.187000000E–12	.187000000E–12
4	lj	.000000000E+00	.000000000E+00
5	pj	.000000000E+00	.000000000E+00
6	–dk	–.311000000E–05	–.260450000E–05
7	hjk	–.967000000E–11	–.967000000E–11
8	ljk	.000000000E+00	.000000000E+00
9	pjk	.000000000E+00	.000000000E+00
10	hk	.217000000E–08	.217000000E–08
11	lkj	.000000000E+00	.000000000E+00
12	pkj	.000000000E+00	.000000000E+00
13	lk	.000000000E+00	.000000000E+00
14	pkjk	.000000000E+00	.000000000E+00
15	pk	.000000000E+00	.000000000E+00
16	E	.107430756E+04	.100845277E+04
17	(B+C)/2	.415825765E+00	.414959680E+00
18	–Dj	–.448000000E–06	–.453803000E–06
19	Hj	.327000000E–12	.327000000E–12
20	Lj	.000000000E+00	.000000000E+00
21	Pj	.000000000E+00	.000000000E+00
22	A–(B+C)/2	.287463043E+01	.282862002E+01
23	–Djk	.132000000E–05	.138740000E–05
24	Hjk	–.300000000E–11	–.300000000E–11
25	Ljk	.000000000E+00	.000000000E+00
26	Pjk	.000000000E+00	.000000000E+00
27	–Dk	–.181000000E–03	–.178366000E–03
28	Hkj	–.158000000E–08	–.996000000E–09
29	Lkkj	.000000000E+00	.000000000E+00
30	Pjjk	.000000000E+00	.000000000E+00
31	Hk	.313000000E–07	.308200000E–07
32	Lkj	.000000000E+00	.000000000E+00
33	Pkkj	.000000000E+00	.000000000E+00
34	Lk	.000000000E+00	.000000000E+00
35	Pkj	.000000000E+00	.000000000E+00
36	Pk	.000000000E+00	.000000000E+00

Coriolis coupling parameters

1	Cy/2	–.230680000E+00
2	C011	–.106320000E–01
3	C021	.000000000E+00
4	C201	.000000000E+00
5	C031	.000000000E+00
6	C211	.000000000E+00
7	C041	.000000000E+00
8	C221	.000000000E+00
9	C401	.000000000E+00
10	C051	.000000000E+00
11	C231	.000000000E+00
12	C411	.000000000E+00
13	C003	.000000000E+00
14	C013	.000000000E+00
15	C023	.000000000E+00
16	C203	.000000000E+00
17	C033	.000000000E+00
18	C213	.000000000E+00
19	C005	.000000000E+00
20	C015	.000000000E+00

Table 3. Spectroscopic parameters (cm^{-1}) of effective rotational Hamiltonian H$_V^{Wats}$ (5) for the (020) state of ^{16}O$_3$ molecule[38]

Parameter number	Parameter	Value
1	′(B–C)/4	.1316355221E–01
2	′dj	.6866370000E–07
3	′dk	.4561185295E–05
4	′hk	.4764705000E–08
5	′hjk	–.2678000000E–10
6	′hj	.2382400000E–12
7	′lk	–.9530000000E–12
8	′lkj	.0000000000E+00
9	′ljk	.0000000000E+00
10	′lj	.0000000000E+00
11	′pk	.0000000000E+00
12	′pkjk	.0000000000E+00
13	′pkj	.0000000000E+00
14	′pjk	.0000000000E+00
15	′pj	.0000000000E+00
16	′qk	.0000000000E+00
17	′qkj	.0000000000E+00
18	′qkkj	.0000000000E+00
19	′qjjk	.0000000000E+00
20	′qjk	.0000000000E+00
21	′qj	.0000000000E+00
1	E	.1399272630E+04
2	(B+C)/2	.4164084144E+00
3	A–(B+C)/2	.3245997770E+01
4	Dk	.2560770500E–03
5	Djk	–.1721188000E–05
6	Dj	.4600638000E–06
7	Hk	.6101600000E–07
8	Hkj	–.2541860000E–08
9	Hjk	.1858500000E–10
10	Hj	.1184500000E–12
11	Lk	–.3334600000E–10
12	Lkj	.0000000000E+00
13	Lkkj	.0000000000E+00
14	Ljk	.0000000000E+00
15	Lj	.0000000000E+00
16	Pk	.4010000000E–13
17	Pkj	.0000000000E+00
18	Pkkj	.0000000000E+00
19	Pjjk	.0000000000E+00
20	Pjk	.0000000000E+00
21	Pj	.0000000000E+00
22	Qk	.0000000000E+00
23	Qkj	.0000000000E+00
24	Qkkj	.0000000000E+00
25	Qkkjj	.0000000000E+00
26	Qjjk	.0000000000E+00
27	Qjk	.0000000000E+00
28	Qj	.0000000000E+00

can be found in the "Help" section of SPECTRA called through right-hand case of the principal menu.

In order to view a chosen parameter set, one should click on right end button ("action"). A result corresponds to the window in Fig. 3, which shows the transition moment parameters for ν_1 and ν_3 bands of ^{16}O^{18}O^{16}O molecule.[35] The ν_1 band parameters correspond to Eq. (3) and those of ν_3 to Eq. (2).

A choice of the "Select" button (Fig. 2) for a chosen band activates the page "Parameters", which offers a choice of a lower and upper states and

conditions for the spectrum computation. Figure 4 shows this page for an example corresponding to the $2\nu_2$ band of $^{16}O_3$ with transition moment parameters taken from Ref. 36. Three sets of the upper state (020) parameters are available in Refs. 36–38, and two sets of the lower state (000) parameters are available in Refs. 37

and 39. The user has an access to a file of parameters via the button "action" in the corresponding string. Tables 2 and 3 give examples for parameter sets of (100) and (001) states of the $^{16}O^{18}O^{16}O$ molecule (Table 2) and (020) of the $^{16}O_3$ molecule (Table 3) as is displayed in the system.
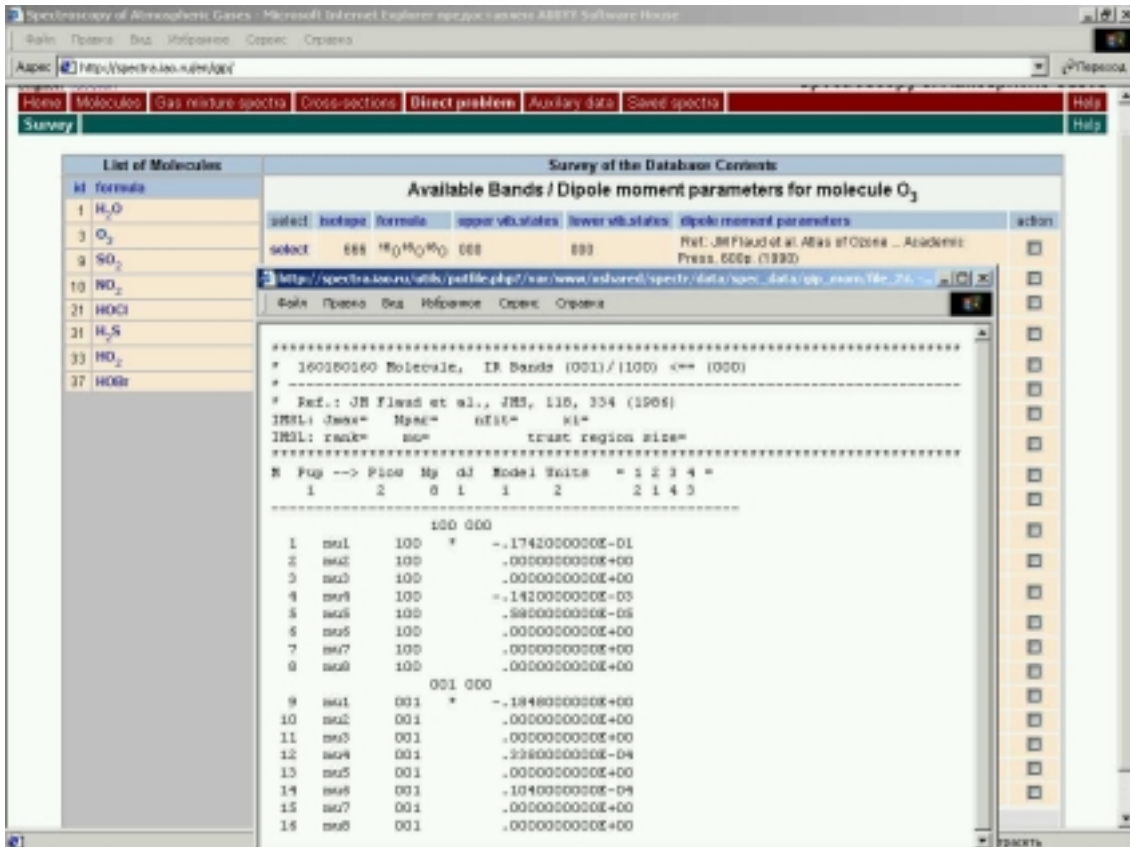

Fig. 3. Effective dipole moment parameters (in debay) for the ν_1 and ν_3 bands of $^{16}O^{18}O^{16}O$ molecule.
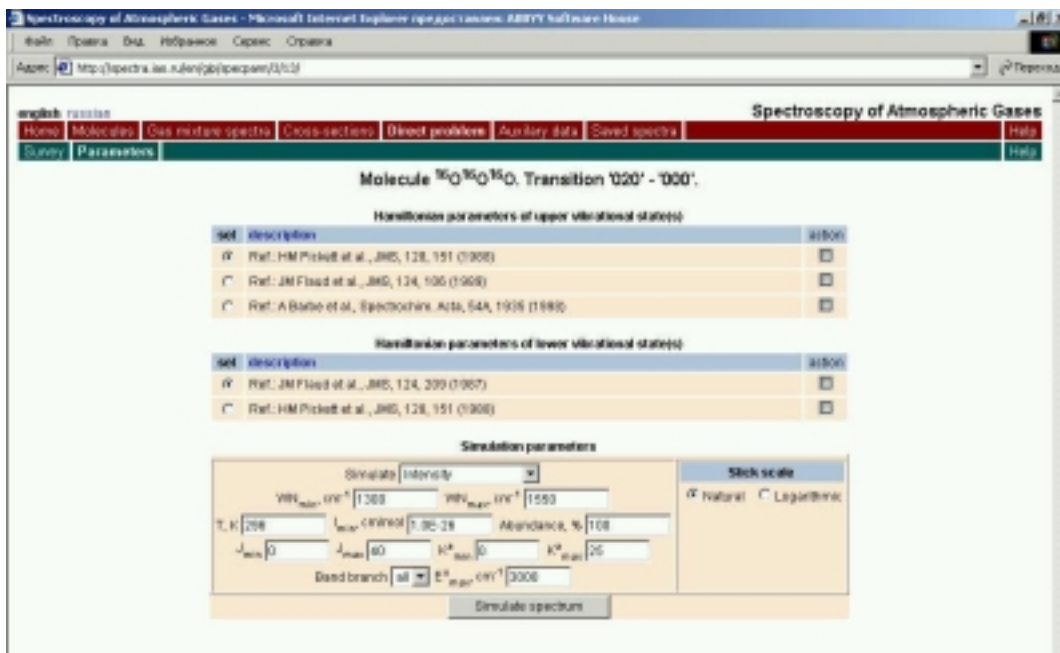

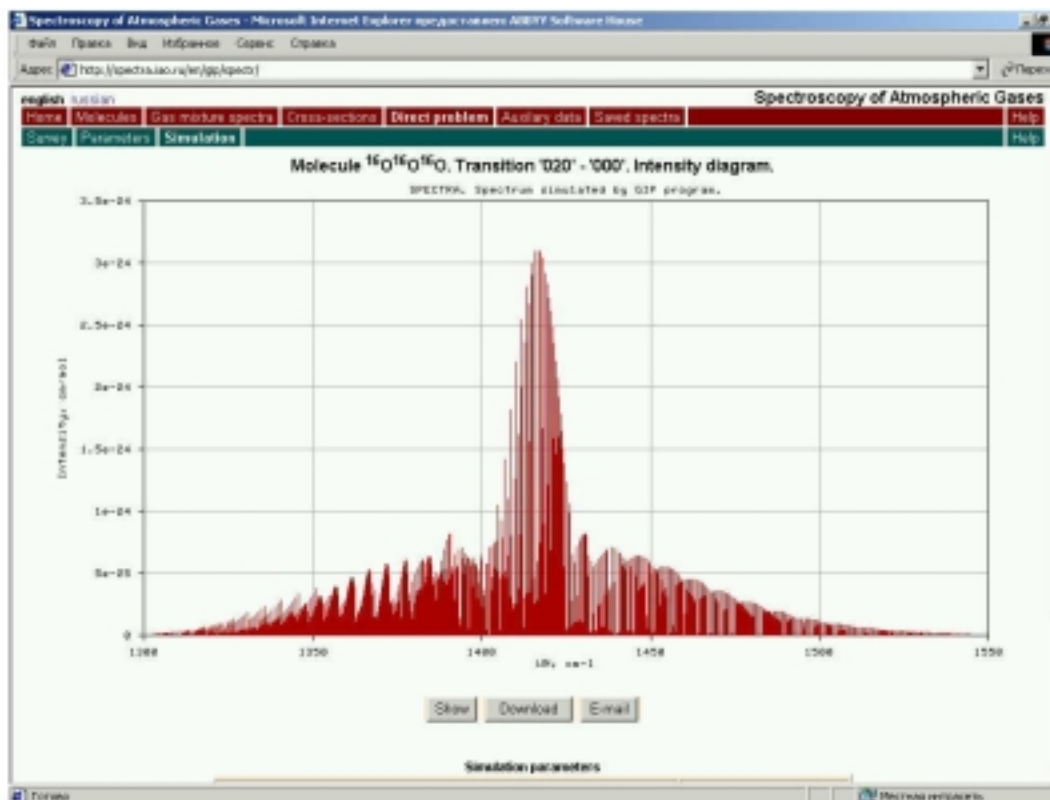**Fig. 4.** Panel of direct task parameters for chosen band.

Fig. 5. Example of simulated spectrum for the $2\nu_2$ band of $^{16}O_3$ molecule.

At the bottom of the "Parameters" page one finds the panel "Simulation parameters". To run a calculation, one needs to set up the following parameters: a) subject of calculations − intensities or transition moments (corresponding to the square of matrix elements of the operator (1)), b) spectral range defined by its lower WN_{min} and upper WN_{max} limits (cm^{-1}), c) temperature T (K), d) cut-off intensity I_{min} (cm^{-1}/mol/cm^{-2}) eliminating weaker lines from a computed list, e) range for rotation quantum numbers J and K_a, f) selection of branches, g) cut-off for energy of VR levels E^u_{max} (cm^{-1}).

On setting all parameters, one must click on the button "Simulate spectrum" in the bottom of the panel. If all parameters were set up correctly, the calculation result is graphically displayed in the window "Simulation" as it is shown in Fig. 5. The result can be also shown as a text in the browser window, or loaded to the user's computer in ZIP format, or send to the user via e-mail through clicking on buttons "Show", "Download", or "E-mail", respectively. Table 4 shows a fragment of an output file for computed $2\nu_2$ band of $^{16}O_3$.

Table 5 displays an example of spectroscopic parameters of the Hamiltonian $\mathbf{H}^G_{rot}$ defined by Eqs. (6)–(8), which have been used for calculations of VR levels of (010) state of H$_2^{16}$O (Ref. 12). The first 23 parameters correspond to the non-diagonal parameters u_{nm} of Eq. (6). Next 5 parameters B0 − B4 refer to the definition of the elementary generating function (8)–(8a) for the non-diagonal part of $\mathbf{H}^G_{rot}$, and parameters A0 − A4 correspond to the elementary generating function (7)–(7a). The last 29 parameters (from 35th to 63rd) are diagonal parameters of Eq. (6). Parameters in Table 5 are listed in the same form as they are presented in the system.

Table 4. Example of the spectra simulation in the ASCII format. Frequencies Fcalc and energies of lower states Elower are in cm^{-1}, intensities are in cm/molec

```
# CALCULATED LINES
# J_min − J_max            0        40
# Ka_min − Ka_max          0        25
# |dKa|_min − |dKa|_max    0         5
# F_min − F_max     1300.0000       1550.0000 cm−1
# Eupper_max        3000.0000 cm−1
# Temperature         296.00 K
# Partition function  3473.000
# Abundance           0.10000000E+01
# Intensity cutoff    0.1E-25 cm/mol
```

Table 4 continued

#	Fcalc	Icalc	v	J	Ka	Kc	v	J	Ka	Kc	Elower
	1395.32441	9.18E-26	020	0	0	0	000	1	1	1	3.94822
	1403.32485	9.59E-26	020	1	1	1	000	0	0	0	0.00000
	1400.80538	3.49E-26	020	1	1	1	000	2	0	2	2.51948
	1388.27290	1.40E-25	020	1	1	1	000	2	2	0	15.05196
	1397.82220	6.26E-26	020	2	0	2	000	1	1	1	3.94822
	1410.80342	1.29E-26	020	2	2	0	000	1	1	1	3.94822
	1396.04110	2.50E-25	020	2	0	2	000	2	1	1	5.72931
	1409.02232	5.89E-26	020	2	2	0	000	2	1	1	5.72931
	1393.74873	1.45E-25	020	2	0	2	000	3	1	3	8.02168
	1381.52519	2.31E-25	020	2	2	0	000	3	3	1	33.22644
	1402.57631	2.11E-25	020	2	1	1	000	2	0	2	2.51948
	1390.04383	9.66E-26	020	2	1	1	000	2	2	0	15.05196
	1387.52434	1.40E-25	020	2	1	1	000	3	2	2	17.57144
	1411.52013	1.59E-25	020	3	2	2	000	2	1	1	5.72931
	1409.22776	9.81E-26	020	3	2	2	000	3	1	3	8.02168
	1384.02299	1.07E-25	020	3	2	2	000	3	3	1	33.22644
	1405.46485	1.54E-26	020	3	2	2	000	4	1	3	11.78459
	1380.66160	2.16E-25	020	3	2	2	000	4	3	1	36.58784
	1404.83739	2.31E-25	020	3	1	3	000	2	0	2	2.51948
	1392.30491	2.40E-26	020	3	1	3	000	2	2	0	15.05196
	1418.41137	1.89E-25	020	3	3	1	000	2	2	0	15.05196
	1389.78542	1.63E-25	020	3	1	3	000	3	2	2	17.57144
	1415.89188	4.60E-26	020	3	3	1	000	3	2	2	17.57144
	1398.96585	8.22E-26	020	3	1	3	000	4	0	4	8.39102
	1386.41666	1.34E-25	020	3	1	3	000	4	2	2	20.94021
	1374.97775	3.08E-25	020	3	3	1	000	4	4	0	58.48558

Table 5. Spectroscopic parameters (in cm^{-1}) of effective rotational Hamiltonian H_{rot}^G for the (010) state of $H_2^{16}O$ molecule[12]

#	Parameter	Value
1	2	3
1	u00	.1389409250E+01
2	u10	−.5746871189E−03
3	u20	.3345282264E−06
4	u30	−.1699700902E−09
5	u40	.0000000000E+00
6	u50	.0000000000E+00
7	u01	−.3889392060E−02
8	u11	−.5066457617E−05
9	u21	.0000000000E+00
10	u31	.0000000000E+00
11	u41	.0000000000E+00
12	u02	.3864801650E−04
13	u12	.4349659887E−06
14	u22	−.2285548296E−09
15	u32	.0000000000E+00
16	u03	.0000000000E+00
17	u13	−.8118110686E−08
18	u23	.6522504445E−11
19	u04	.1928546455E−07
20	u14	.0000000000E+00
21	u24	.1732647204E−13
22	u05	−.7205705520E−10
23	u06	.0000000000E+00
24	B0	.1264542019E+00
25	B1	.1503764037E−03
26	B2	−.9171474669E−06
27	B3	.1878822756E−08
28	B4	.0000000000E+00
29	A0	.5253981301E−01
30	A1	.1392382332E−03

Table 5 continued

1	2	3
31	A2	.0000000000E+00
32	A3	.3019349325E−10
33	A4	−.1170253112E−12
34	A5	.0000000000E+00
35	g00=E	.1594750919E+04
36	g10	.1190770989E+02
37	g20	−.1389339775E−02
38	g30	.6031676120E−06
39	g40	−.2246213731E−09
40	g50	.0000000000E+00
41	g01	.1922058788E+02
42	g11	.7853028298E−02
43	g21	.9334563451E−06
44	g31	.2199451063E−07
45	g41	−.3048077801E−10
46	g51	.0000000000E+00
47	g02	.1942131492E+00
48	g12	.7152834391E−03
49	g22	−.1301877907E−06
50	g32	−.4258289456E−09
51	g42	.2578465647E−12
52	g03	−.1129331174E−02
53	g13	−.3909585803E−05
54	g23	.2082164254E−08
55	g33	.0000000000E+00
56	g04	.1645238296E−05
57	g14	.0000000000E+00
58	g24	.0000000000E+00
59	g05	.8297692198E−08
60	g15	.0000000000E+00
61	g06	.0000000000E+00
62	g07	.0000000000E+00
63	g08	.0000000000E+00

Conclusion

This paper gives a detailed description for one of user-accessible computational function of the information system SPECTRA ("Spectroscopy of Atmospheric Gases"). The system offers an Internet access to data corresponding to well-known spectroscopic line data banks HITRAN[2] and GEISA[4] and to some original data obtained in the Institute of Atmospheric Optics SB RAS and through a cooperation with other research teams.

Note that one of important features of the present system is a possibility of an interactive interface for a solution of various problems of molecular spectroscopy, in particular, for modeling high-resolution and low-resolution molecular spectra. A "Direct problem" function offers the user a possibility to extent spectra computation to intervals of his own interest in those cases, when they are not sufficiently represented in other accessible databases of line parameters. A possibility to download the results to the user's computer for a further treatment represents a certain interest.

Acknowledgments

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